Ethyl orthoformate 122-51-0 | DTXSID8041957

Model Performance

Model	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 4.14 days

Global applicability domain: Outside

Local applicability domain index: 1.81e-01

Confidence level: 8.09e-01

Nearest Neighbors from the Training Set

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2-Methylhexane Measured: 12.5 Predicted: 5.54 Image not found

3-Methylhexane Measured: 157 Predicted: 6.83 Image not found

2-Methylheptane Measured: 12.5 Predicted: 3.99

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Pentane Measured: 40.7 Predicted: 6.52